

Kink Localization under Asymmetric Double-Well Potential

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We study diffuse phase interfaces under asymmetric double-well potential energies with degenerate minima and demonstrate that the limiting sharp profile, for small interface energy cost, on a finite space interval is in general not symmetric and its position depends exclusively on the second derivatives of the potential energy at the two minima (phases). We discuss an application of the general result to porous media in the regime of solid-fluid segregation under an applied pressure and describe the interface between a fluid-rich and a fluid-poor phase.

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I. INTRODUCTION

Quench a system from the homogeneous phase into a broken-symmetry one (think, e.g., to a ferromagnet or to a gas abruptly cooled below their critical temperature). The two phases have to separate and the process can be described via a local field u (local magnetization in ferromagnets, density in liquid-vapor systems, concentration in alloys, etc.) on the physical space $\Omega \subset \mathbb{R}^d$.

Very well known models [1] for the description of the field evolution are the Allen-Cahn and the Cahn-Hilliard equations. With suitable boundary conditions the former is an appropriate equation when the order parameter, i.e., the integral over Ω of the field u , is not conserved, while the latter applies in the conserved case. On mathematical grounds, these equations can be thought as the gradient equation $\partial u / \partial t = -\delta F / \delta u$, in a suitable Hilbert space [2–4], for the *Landau energy functional*

$$F[u] = \int_{\Omega} \left[\frac{1}{2} k^2 \|\nabla u\|^2 + V(u) \right] dx \quad (1)$$

with $k > 0$ and the *potential energy* V a double well positive regular function with degenerate zero value absolute minima in a, b , called *phases* of the system. More precisely, if no constraint to the order parameter is imposed, it is possible to compute the gradient of the Landau functional in the Hilbert space $L^2(\Omega)$ to get the Allen-Cahn equation [4, equations (8) and (12)]. When the integral of

the field u is assumed to be constant throughout the evolution, computing the gradient in the $L^2(\Omega)$ results into a non-local evolution equation, while by using the Hilbert space $H^{-1}(\Omega)$ the Cahn-Hilliard equation is found [4, equation (91) and the comment below equation (90)].

In this paper we discuss some properties of the stationary profile connecting the two phases a and b , namely, the profile which is reached by the system at infinite time. More precisely, we explore the properties of the stationary profile connecting the two phases when the double well potential energy is asymmetric. The equations for the interface profile are the Euler-Lagrange equations for the stationary points of the energy functional (1). These kind of problems are often referred to in the literature as *gradient* or *diffuse interface* problems [5].

We shall consider a one-field u system described by a potential energy V as above. More precisely we shall assume, throughout the paper, that the following condition is satisfied.

Condition 1 *The function $V : \mathbb{R} \rightarrow \mathbb{R}$ is a positive $C^2(\mathbb{R})$ function with two single isolated local minima a and b (assume $a < b$) and such that $V(a) = V(b) = 0$, $V''(a) > 0$, and $V''(b) > 0$.*

Under this assumption, we shall approach the phase interface problem in dimension one, on a finite interval with Dirichlet boundary conditions fixing the values of the two phases at the extreme points of the interval to a and b , respectively. We prove that, for small k , the position of the interface depends exclusively on the second derivatives of the potential energy V at the minima a and b . In particular, the statement is valid for the sta-

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tionary solutions of the Allen-Cahn equation at imposed zero chemical potential and for those of the Cahn-Hilliard equation at imposed zero Lagrange multiplier (for mass conservation).

Note that even if V is not symmetric, the interface falls in the middle point of the space interval provided the two second derivatives are mutually equal.

The interest to study the interface problem in the case of an asymmetric double-well potential energy is due to the fact that they appear naturally in different physical situations. For example, in [3, 6–8] we introduced a model describing a pressure guided transition between a fluid-rich and a fluid-poor phase and based on an asymmetric double-well potential energy. In this theory two order parameters m and ε are introduced, having respectively the physical meaning of fluid density and solid strain. In [3, 7] the interface separating the two coexisting phase has been studied and it has been shown that its localization properties, due to the asymmetry of the potential energy, are not trivial.

Apart from the application mentioned above, due to its general character, our result is of interest for any situation in which diffuse interfaces are relevant. In particular when approximate computations or numerical simulations are performed in the regime of small interface energy cost, our rigorous prediction could result valuable in testing the soundness of the results. We remark that in this kind of problems numerical computations become particularly difficult when the interface energy cost is small (say $k \sim 10^{-2}$ with our parametrization).

The paper is organized as follows. In Section II we state our general results. In Section III we discuss in detail their application to the porous media segregation problem. In Section IV we shall verify our result in some cases physically relevant by performing numerical computations. In Section V, finally, we prove the results stated in Section II.

II. RESULTS

We approach the problem in dimension one. Recalling k is a positive constant, the Euler-Lagrange equations for the energy functional (1) reads as the Dirichlet boundary value problem

$$k^2 u_{xx} = V'(u) \quad \text{with } u(0) = a \quad \text{and } u(\ell) = b \quad (2)$$

for the field $u(x)$, $x \in [0, \ell]$, for some $\ell > 0$.

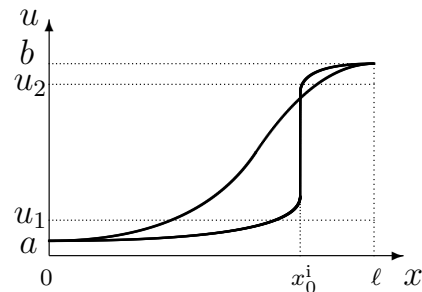


FIG. 1. Schematic description of the results in Theorems 1 and 2. The thick lines are the profiles at two finite values of k ; the steepest one corresponds to the smallest value of k .

From the physical point of view the problem (2) is that of finding the stationary profile connecting the two phases a and b on the finite space interval $[0, \ell]$. We remark that the above problem (2) is found when looking for the stationary solutions of the Allen-Cahn equation at imposed zero chemical potential or of the Cahn-Hilliard equation at imposed zero Lagrange multiplier (for mass conservation) with proper boundary conditions.

Before stating our results, we note that by exploiting the one-dimensionality of the model a phase space analysis [9] proves that the problem (2) has a unique solution implicitly given by the integral

$$\int_a^u \frac{k \, ds}{\sqrt{2[E_k + V(s)]}} = x \quad (3)$$

where for any $k > 0$ we have defined implicitly the energy level E_k by the equation

$$\int_a^b \frac{k \, ds}{\sqrt{2[E_k + V(s)]}} = \ell \quad (4)$$

namely, the integral in (3) with $u = b$ and $x = \ell$.

We note that the solution of (3) is a kink connecting on the interval $[0, \ell]$ the phase a to the phase b . At small k the energy cost associated with the gradient of u , see (1), is small, so that the interface width is of order k and it is localized somewhere in the interval $[0, \ell]$. This remark is made rigorous in the next classical theorem, where we state that in the limit $k \rightarrow 0$ the interface tends to a discontinuous kink connecting the two phases (see, also, figure 1).

Theorem 1 *Assume Condition 1 is satisfied. Then, for any $u_1, u_2 \in (a, b)$ such that $u_1 < u_2$*

$$\lim_{k \rightarrow 0} \int_{u_1}^{u_2} \frac{k \, ds}{\sqrt{2[E_k + V(s)]}} = 0 \quad (5)$$

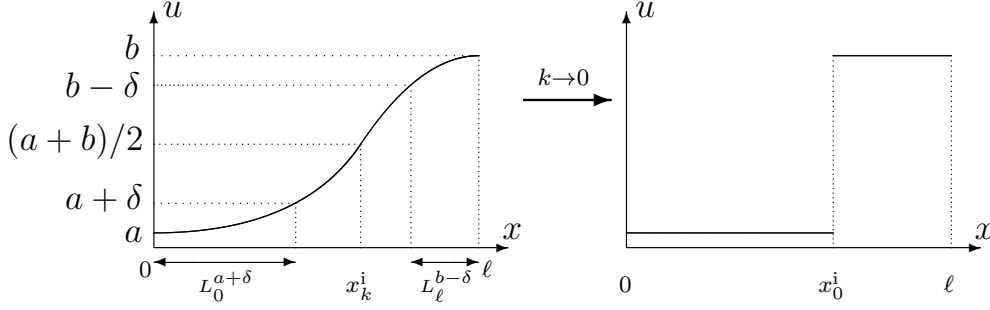


FIG. 2. Schematic description of the heuristic interpretation of equation (7). The thick line is the profile at finite k , whereas the thin discontinuous line is its $k \rightarrow 0$ limit.

The meaning of the theorem above is illustrated in figure 1. For any choice of $a < u_1 < u_2 < b$, by choosing k small enough the distance between the two points where the kink attains the values u_1 and u_2 respectively can be made smaller than any fixed positive number.

The theorem above suggests that for any $k > 0$, it is meaningful to define the *interface position* x_k^i as that (unique) point where the profile attains the value $(a + b)/2$, that is to say

$$x_k^i = \int_a^{\frac{a+b}{2}} \frac{k \, ds}{\sqrt{2[E_k + V(s)]}} \quad (6)$$

Since for $k \rightarrow 0$ the profile tends to a step function, different definitions, equivalent in this limit, are possible for the interface position; e.g., the point where the profile equals the value of field corresponding to the local maximum of the potential energy.

The following theorem gives the limiting behavior of the interface position for $k \rightarrow 0$.

Theorem 2 *Assume Condition 1 is satisfied. Then*

$$\lim_{k \rightarrow 0} [\sqrt{V''(a)} x_k^i - \sqrt{V''(b)} (\ell - x_k^i)] = 0 \quad (7)$$

In words, the theorem states that in the limit $k \rightarrow 0$ the distance of the interface from the boundary points is proportional to the inverse of the square root of the second derivative of the potential energy evaluated at the corresponding minimum of V . Note that from (7) it follows immediately that the interface position x_k^i for $k \rightarrow 0$ tends to

$$x_0^i = \frac{\ell \sqrt{V''(b)}}{\sqrt{V''(a)} + \sqrt{V''(b)}} \quad (8)$$

The limiting interface position x_0^i depends only on the second derivatives of the potential energy evaluated at

the minima. In particular if $V''(a) = V''(b)$ then $x_0^i = \ell/2$, that is to say, the interface is located at the middle point of the interval $[0, \ell]$.

The proof (see Section V) of (7) is based on a direct evaluation of the integral (6). Since E_k is small for $k \rightarrow 0$ the integrand diverges in a . The integral can be thus estimated by expanding in Taylor formula to the second order the potential energy V .

Now, we give two heuristic arguments supporting the statement of the theorem. In Section IV, on the other hand, we shall verify the result with some numerical computations in two cases of interest.

Assuming k small, the kink is close to a step function. By phase space techniques it follows $E_k \approx 0$. Fix $\eta > 0$ small and $\eta < \delta \ll b - a$. By (3) the distance between the points where the profile equals $a + \eta$ and $a + \delta$ is

$$\int_{a+\eta}^{a+\delta} \frac{k \, ds}{\sqrt{2[E_k + V(s)]}} \approx \int_{a+\eta}^{a+\delta} \frac{k \, ds}{\sqrt{V''(a)(u-a)}}$$

where we have neglected E_k and, noted that the integral is extend to a very small interval close to a , we expanded V in second order Taylor formula. Since η is small, we have that the distance $L_0^{a+\delta}$ from 0 of the point where the value $a + \delta$ is attained by the profile is approximatively given by $L_0^{a+\delta} \approx (k/\sqrt{V''(a)}) \log(\delta/\eta)$.

By performing a similar computation in the neighborhood of the boundary point ℓ and with obvious notation we get $L_\ell^{b-\delta} \approx (k/\sqrt{V''(b)}) \log(\delta/\eta)$. The last two formulas allow to conjecture the validity of (7), see also figure 2.

The second heuristic argument is based on the interpretation of (2) as the equation describing the motion of a particle of mass k^2 under the potential energy $-V$. In this language u is the position of the particle and x is the time. In the remaining part of this section, thus, we

shall address to $u(x)$ as to the position of the particle at time x and, for this reason, derivatives with respect to x will be denoted by dots.

In this context, solving (2) means looking for the motion started at a with positive initial velocity v_0 such that at time ℓ the position b is reached. The conservation of the total mechanical energy $k^2\dot{u}^2/2 - V(u)$ implies that the motion will reach the point b with velocity v_0 . The interface position x_k^i is then the time at which the particle reaches the position $(a+b)/2$.

We can describe such a motion by linearizing the equation of motion in a neighborhood of the two unstable equilibrium points a and b . We get

$$k^2\ddot{u} = V''(a)(u-a) \quad \text{and} \quad k^2\ddot{u} = V''(b)(u-b)$$

respectively. We then solve the two equations with the initial conditions $(u(0), \dot{u}(0)) = (a, v_0)$ and $(u(0), \dot{u}(0)) =$

$(b, -v_0)$, respectively, and get

$$u_a(x) = a + \frac{kv_0}{\sqrt{V''(a)}} \sinh\left(\frac{\sqrt{V''(a)}}{k}x\right)$$

for the motion started at a and

$$u_b(x) = b - \frac{kv_0}{\sqrt{V''(b)}} \sinh\left(\frac{\sqrt{V''(b)}}{k}x\right)$$

for the motion that started at b .

Recalling that x_k^i is the time at which the particle is at $(a+b)/2$, by the two equation above we get

$$x_k^i = \frac{k}{\sqrt{V''(a)}} \operatorname{arcsinh}\left(\frac{b-a}{2} \frac{\sqrt{V''(a)}}{kv_0}\right)$$

and

$$\ell - x_k^i = \frac{k}{\sqrt{V''(b)}} \operatorname{arcsinh}\left(\frac{b-a}{2} \frac{\sqrt{V''(b)}}{kv_0}\right)$$

Recalling that $\operatorname{arcsinh}(x) = \log(x + \sqrt{x^2 + 1})$, with simple algebra we get

$$\sqrt{V''(a)}x_k^i - \sqrt{V''(b)}(\ell - x_k^i) = k \left[\log \frac{\sqrt{V''(a)}(b-a) + \sqrt{V''(a)(b-a)^2 + 4k^2v_0^2}}{\sqrt{V''(b)}(b-a) + \sqrt{V''(b)(b-a)^2 + 4k^2v_0^2}} \right] \quad (9)$$

which suggests the validity of (8) since the right hand side tends to zero for $k \rightarrow 0$. Note that v_0 does not diverge for $k \rightarrow 0$.

III. PHASE INTERFACE IN POROUS MEDIA

We discuss, now, in detail the application of the above results to the study of transitions from a fluid-poor towards a fluid-rich phase in porous media under consolidation. The model we study here is supposed to explain the behavior of the system in consolidation regime, namely, when an external pressure is applied on the solid component. The idea is that of explaining the existence of two phases, differing in liquid content, due to the modification in the solid structure caused by the external pressure. For this reason, as in the original Biot theory, in this model no chemical potential contribution is considered.

In [3, 7] the interface separating the two coexisting phases has been studied numerically and it has been shown that its localization properties, due to the asymmetry of the potential energy, are not trivial. In fig-

ures 3–6 profiles for the solid strain ε and the fluid density m fields are shown. It is immediate to note that those kinks tend, for the interface energy cost tending to zero, to a not symmetric sharp interface between the two phases.

More precisely, in this model three interface cost parameters, k_1 , k_2 , and k_3 , are introduced (see equation (11) below). These constants weights $(\varepsilon')^2$, $\varepsilon'm'$, and $(m')^2$, respectively. The numerical simulations suggest that when $k_1, k_2, k_3 \rightarrow 0$ with mutual ratios kept constant, the interface tends to a definite position not depending on these ratios. The ε and the m profiles are shown in the cases $k_1 = k_2 = k_3$ in figures 3 and 4 and $k_1 = 2k_2 = 3k_3$ in figures 5 and 6, respectively.

In Section II we have proven results concerning the localization properties of a kink connecting two coexisting phases in a quite general one-field one-dimensional setup. As a straightforward application, we shall get the position of the limiting interface for the poromechanics model described above with the second gradient coefficients such that $k_1k_3 - k_2^2 = 0$; in this particular case,

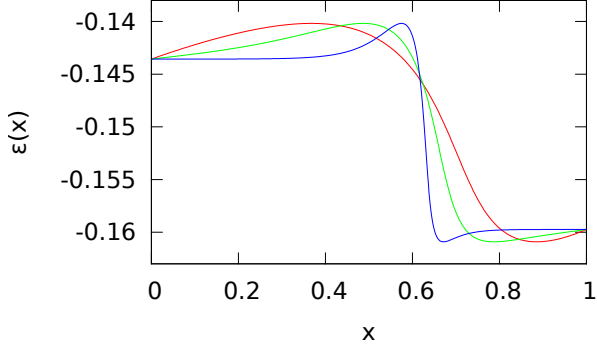


FIG. 3. Kink profiles for the strain field ε for the potential energy (11)–(13) with $k_1 = k$, $k_2 = k$, $k_3 = k$, $k = 10^{-1}, 10^{-2}, 10^{-3}$, $\alpha = 100$, $a = 1/2$, and $b = 1$.

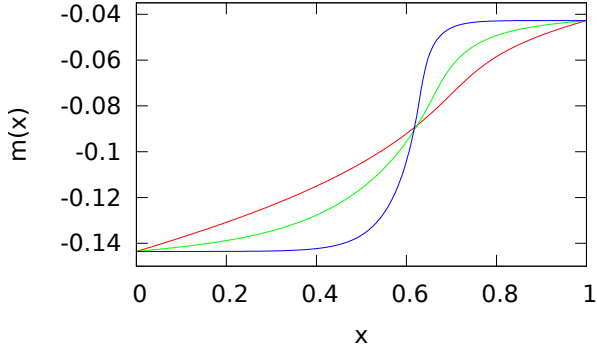


FIG. 4. Kink profiles for the fluid density field m for the same parameters as in figure 3.

indeed, the two-field model will reduce to a one-field one.

For the complete description of the poromechanics setup we refer the readers to [3, 7, 8, 10]. We recall that two fields $m, \varepsilon : [0, \ell] \rightarrow \mathbb{R}$ are introduced having the physical meaning of deviation from a reference value of the fluid density and solid strain, respectively. The stationary state of the system is described by the Euler–Lagrange equations, with suitable boundary conditions, for the variational problem associated with the Landau energy functional

$$L[m, \varepsilon] = \int_0^\ell [K(m', \varepsilon') + \Psi(m, \varepsilon)] dx \quad (10)$$

where K and Ψ are, respectively, called the *second* and *first* gradient potential energy.

The poromechanics model we study in this paper [8] is defined by choosing the second and the first gradient potential energies as follows. We let

$$K(m', \varepsilon') = \frac{1}{2} [k_1 (\varepsilon')^2 + 2k_2 \varepsilon' m' + k_3 (m')^2] \quad (11)$$

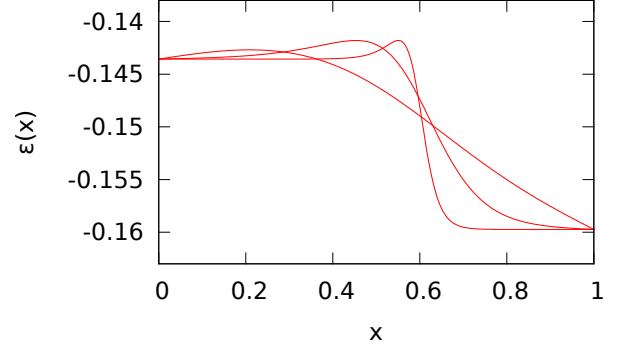


FIG. 5. Kink profiles for the strain field ε for the potential energy (11)–(13) with $k_1 = k$, $k_2 = k/2$, $k_3 = k/3$, $k = 10^{-1}, 10^{-2}, 10^{-3}$, $\alpha = 100$, $a = 1/2$, and $b = 1$.

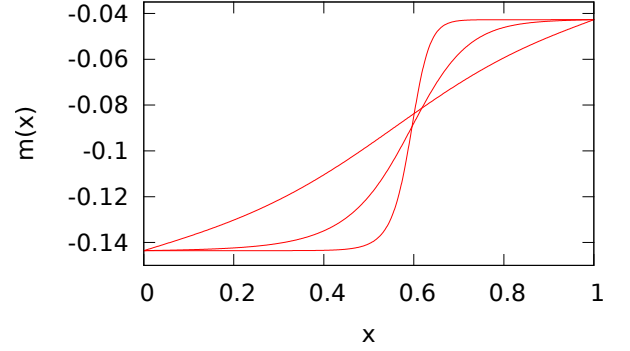


FIG. 6. Kink profiles for the fluid density field m for the same parameters as in figure 5.

where $k_1, k_3 > 0$ and $k_2 \in \mathbb{R}$ are such that $k_1 k_3 - k_2^2 \geq 0$ and the prime denotes the space derivative. Moreover we set

$$\Psi(m, \varepsilon, p) = \frac{\alpha}{12} m^2 (3m^2 - 8b\varepsilon m + 6b^2 \varepsilon^2) + \Psi_B(m, \varepsilon, p) \quad (12)$$

where

$$\Psi_B(m, \varepsilon, p) = p\varepsilon + \frac{1}{2} \varepsilon^2 + \frac{1}{2} a(m - b\varepsilon)^2 \quad (13)$$

is the Biot potential energy density [11], $a > 0$ is the ratio between the fluid and the solid rigidity, $b > 0$ is a coupling between the fluid and the solid component, $p > 0$ is the external pressure, and $\alpha > 0$ is a material parameter responsible for the showing up of the additional equilibrium. We remark that the condition $k_1 k_3 - k_2^2 \geq 0$ ensures that the second gradient part K of the overall potential energy density is convex. Under this assumption there exists a minimizer for the action functional (10) on a bounded domain [12].

In [6, 8] we have studied the minima of the potential

energy (12) and shown that they can be interpreted as the homogeneous *phases* of the system. We have proven that there exists a pressure p_c , called *critical pressure*, such that for any $p \in [0, p_c)$ there exists a single phase $(m_s(p), \varepsilon_s(p))$, called the *standard phase*, which is very similar to the usual solution of the Biot model. For $p > p_c$ a second phase $(m_f(p), \varepsilon_f(p))$, richer in fluid with respect to the standard phase and hence called *fluid-rich* phase, appears. It has also been shown that for any $p > 0$ the point $(m_s(p), \varepsilon_s(p))$ is a local minimum of the two variable potential energy $\Psi(m, \varepsilon)$ with p fixed, while $(m_f(p), \varepsilon_f(p))$ is a local minimum for $p > p_c$ and a saddle point for $p = p_c$.

Moreover, in [7] it has been proven that there exists a unique value p_{co} of the pressure, called *coexistence pressure*, such that the potential energy of the two phases is equal. More precisely, it has been proven that the equation $\Psi(m_s(p), \varepsilon_s(p)) = \Psi(m_f(p), \varepsilon_f(p))$ has the single solution p_{co} . We remark that it is not possible to provide explicit formulas for the phase field values and for the coexistence pressure. Indeed, these quantities do depend on the physical parameters of the model α , a , and b . In [7, 8] we have proved (uniformly in these parameters) the scenario depicted above and we have provided

a strategy for the numerical determination of all the interesting quantities.

The behavior of the system at the coexistence pressure is particularly relevant; from now on we shall always consider $p = p_{co}$ and, for this reason, we shall drop p from the notation. When the external pressure is equal to p_{co} , none of the two above phases is favored and we ask if profiles connecting one phase to the other exist [3]. In [7] this problem has been addressed on the space set \mathbb{R} , while some results on a finite interval have been reported in [3]. There we have remarked that the localization properties of the kink profile are not trivial, as it has been fully explained above.

The profiles connecting the two phases on a finite interval $[0, \ell]$ at the coexistence pressure are given by the solutions (if any) of the Dirichlet boundary problem for the Euler–Lagrange equations associated with the functional (10), namely

$$\frac{\partial \Psi}{\partial \varepsilon} - \frac{d}{dx} \frac{\partial K}{\partial \varepsilon'} = 0 \quad \text{and} \quad \frac{\partial \Psi}{\partial m} - \frac{d}{dx} \frac{\partial K}{\partial m'} = 0 \quad (14)$$

(see, for instance, [7, equation (4)]), with boundary conditions $m(0) = m_s$, $\varepsilon(0) = \varepsilon_s$, $m(\ell) = m_f$, and $\varepsilon(\ell) = \varepsilon_f$. By writing explicitly the Euler–Lagrange equations we finally get the Dirichlet problem

$$\begin{cases} k_1 \varepsilon'' + k_2 m'' = -(2/3)\alpha b m^3 + \alpha b^2 m^2 \varepsilon + p + \varepsilon - ab(m - b\varepsilon) \\ k_2 \varepsilon'' + k_3 m'' = \alpha m^3 - 2\alpha b m^2 \varepsilon + \alpha b^2 m \varepsilon^2 + a(m - b\varepsilon) \\ m(0) = m_s, \varepsilon(0) = \varepsilon_s, m(\ell) = m_f, \varepsilon(\ell) = \varepsilon_f \end{cases} \quad (15)$$

which can be approached numerically with the finite difference method powered with the Newton–Raphson algorithm. The solution we find, in the cases of interest, are those depicted in the figures 3–6.

As noted above the behavior at small second gradient coefficient k_1 , k_2 , and k_3 , of the stationary profiles depicted in figures 3 – 6 is very peculiar: when $k_1, k_2, k_3 \rightarrow 0$ with mutual ratios kept constant, the interface becomes sharp and its location tends to a definite position not depending on these ratios. Although the general results in Section II do not apply to this case, we note that the solutions of the problem (15) behave in tune with those of the general one-field problem (2).

At the moment, as already mentioned above, we can explain this fact only in the particular case $k_1 k_3 - k_2^2 = 0$, namely, $k_1/k_2 = k_2/k_3$. In this case, called *degenerate*

case in [7], the problem of finding a solution of the stationary problem can be reduced to a one-field problem. Indeed, in such a case one performs the rotation of the Cartesian reference system

$$\xi := \frac{m + \lambda \varepsilon}{\sqrt{1 + \lambda^2}} \quad \text{and} \quad \eta := \frac{-\lambda m + \varepsilon}{\sqrt{1 + \lambda^2}} \quad (16)$$

in the plane m – ε , where $\lambda := k_1/k_2 = k_2/k_3$, and defines

$$U(\xi, \eta) = \Psi(m(\xi, \eta), \varepsilon(\xi, \eta)) \quad (17)$$

Then one shows that the two fields $m(x)$ and $\varepsilon(x)$ are solutions of the two equations (15) if and only if the corresponding fields $\xi(x)$ and $\eta(x)$ satisfy

$$k_3(1 + \lambda^2)\xi'' = \frac{\partial U}{\partial \xi}(\xi, \eta) \quad \text{and} \quad \frac{\partial U}{\partial \eta}(\xi, \eta) = 0 \quad (18)$$

The root locus of the *constraint curve* $\partial U(\xi, \eta)/\partial \eta = 0$ is made of a certain number of maximal components

such that each of them is the graph of a function $\xi \in \mathbb{R} \rightarrow \eta(\xi) \in \mathbb{R}$; for each of them the first between the two equations (18) becomes a one-field one-dimensional problem.

Since the function U has been obtained by rotating the coordinate axes, then at the coexistence pressure it has the two absolute minimum points (ξ_s, η_s) and (ξ_f, η_f) corresponding, respectively, to the standard and to the fluid-rich phases. Since (m_s, ε_s) and (m_f, ε_f) satisfy the equations $\Psi_m(m, \varepsilon) = 0$ and $\Psi_\varepsilon(m, \varepsilon) = 0$, we have that the two points (ξ_s, η_s) and (ξ_f, η_f) are solutions of the constraint equation $\partial U(\xi, \eta)/\partial \eta = 0$ and hence they belong to the constraint curve.

In [7] we have seen that there exist values of the second gradient parameters k_1 , k_2 , and k_3 such that the two points above fall on the same maximal component of the constraint equation. Since, in this case, the function U has two isolated absolute minima which, by hypothesis, belong to the same maximal component of the constraint curve, we have that the function $U(\xi, \eta(\xi))$ of ξ has two absolute isolated minima in ξ_s and ξ_f .

In this particular case, finally, the theory developed in Section II can be applied to the poromechanics problem (15) and the results discussed in the introduction find a complete explanation. The explanation is not only qualitative, but also quantitative, indeed, for the first gradient parameters chosen as in the figures 3 and 4, namely, $\alpha = 100$, $a = 1/2$, and $b = 1$, by computing the second derivatives of the one-field potential energy $U(\xi, \eta(\xi))$ at the phases ξ_s and ξ_f and by using (8) we get 0.6164 for the position of the interface on the interval $[0, 1]$. For the second gradient parameter choice in figures 3 and 4 the degeneracy condition $k_1 k_3 - k_2^2 = 0$ is satisfied. So that in this case the theory developed in Section II applies and the match with the numerical result is striking.

IV. TWO NUMERICAL EXAMPLES

In this section we check numerically (7) for two very well known potentials. The first example, see (19), is an asymmetric potential with mutually different second derivatives at the minima; the numerical computation will confirm that, for k small, the interface is not located at the middle point of the space interval and that its position is given by (8). The second example, see (20), is, on the other hand, an asymmetric potential with mutually equal second derivatives at the minima; the numerical computation will confirm that, for k small, the interface

is located at the middle point of the space interval.

We shall solve the equation (2) with $\ell = 1$ via the following procedure. Fix k and use (4) to compute the energy level E_k ; then use (3) to compute the profile.

We consider first the following asymmetric double-well potential [13, 14]

$$V_1(u) = \frac{1}{\omega_0^2} \left(\frac{1 - \exp[b_1(u-1)]}{1 - \exp[b_1(u_0-1)]} \times \frac{1 - \exp[-b_2(u+1)]}{1 - \exp[-b_2(u_0+1)]} \right)^2 \quad (19)$$

where $\omega_0 \in \mathbb{R}$, $b_1, b_2 > 0$, and $u_0 \in (-1, +1)$. The two minima are at ± 1 and u_0 controls the height of the internal barrier. The kinks corresponding to $k = 1.0, 0.5, 0.25, 0.1$ (for $\omega_0 = 1$, $b_1 = 1$, $b_2 = 5$, $u_0 = 0.5$) are shown in figure 7. By applying (8) one gets $x_0^i = [1 + e^2 + e^4 + e^6 + e^8]/[1 + e^2 + e^4 + e^6 + 6e^8] \approx 0.187846$, so that the numerical computation is in good agreement with the theoretical prediction (8).

Another interesting example is the asymmetric potential which is considered the benchmark potential [15–17] of the current literature on rocked ratchets, namely,

$$V_2(u) = \sigma \sin \left[\frac{2\pi}{a}(u-u_0) \right] + \frac{\sigma}{4} \sin \left[\frac{4\pi}{a}(u-u_0) \right] + R \quad (20)$$

with $a \in \mathbb{R}$, $\sigma^{-1} = (a/(8\pi))(\sqrt{3}/2)^{1/2}(3 + \sqrt{3})$, $u_0 = (a/(2\pi)) \cos^{-1}((-1 + \sqrt{3})/2)$, and $R = -2\pi/a$. The not essential additive constant R in (20) has been introduced in order to ensure that the potential is equal to zero at the minima na with $n \in \mathbb{Z}$. The second derivative of V_2 at the minima na are all equal since the function is periodic with period a . Some algebra yields $V_2''(na) = 16(-1 + \sqrt{3})\pi^3/a^3$, so that these derivatives are not zero. The kinks corresponding to $k = 3.0, 1.5, 1.0, 0.5, 0.45$ (for $a = 1$) are shown in figure 8.

We stress that, in this case, although the potential energy is asymmetric with respect to the phase exchange, the interface tends to be located in the middle point of the space interval, since the second derivatives of the potential energy at the minima are mutually equal.

Note that our result applies even if deformations of the standard rocket ratchet potential (20) are considered (see [18]). For instance the positive multiplicative factor $1/4$ in the second term in (20) can be chosen differently. Our result is still valid, provided no other minima is found between 0 and $a = 1$, since the second derivatives of the potential at the minima are equal and do not vanish.

It is notable to remark the following. In the above sections we have studied the localization properties of

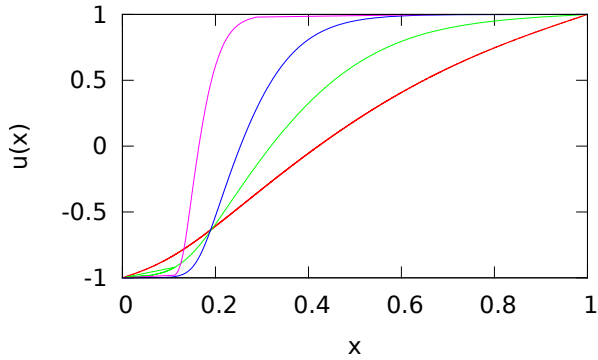


FIG. 7. Graph of the kink for the potential (19) for $\omega_0 = 1$, $b_1 = 1$, $b_2 = 5$, and $u_0 = 0.5$. The profiles correspond to $k = 1.0, 0.5, 0.25, 0.1$ in increasing order of steepness.

the interfaces connecting two phases under an asymmetric double-well potential energy with degenerate minima and we have stated (see Section V for the proof) that the position of the interface depends exclusively on the second derivatives of the potential energies at the two phases.

Although we cannot say, at the moment, to which extent this analogy between the two results can be pushed forward, we note that our result is similar in spirit to those related to the direction of motion of a dc soliton current in ac drive rocket ratchet. Which is, a priori, a completely different problem with respect to the phase interface problem (2) that we have studied.

We refer in particular to [13, 14]. There the authors considered the potential (19) and proved the following: a string soliton profile is pushed by “symmetric” thermal fluctuations sidewise towards the boundary point where the boundary condition has been chosen equal to the phase corresponding to the narrowest valley (biggest second derivative) of the double-well potential. In particular in [14] it is shown that this tendency to move towards the narrowest valley is controlled by the second derivatives of the potential energy evaluated at the phases.

V. PROOF OF RESULTS

The proof of the results in Section II is based on the classical Weierstrass qualitative analysis of the one-dimensional mechanical problem equivalent to (2) [9].

Before starting the proof of the results, we note that E_k is an increasing positive function of k and $E_k \rightarrow 0$ for $k \rightarrow 0$. This is a quite intuitive result since taking the limit $k \rightarrow 0$ is the same as considering a zero mass limit in the

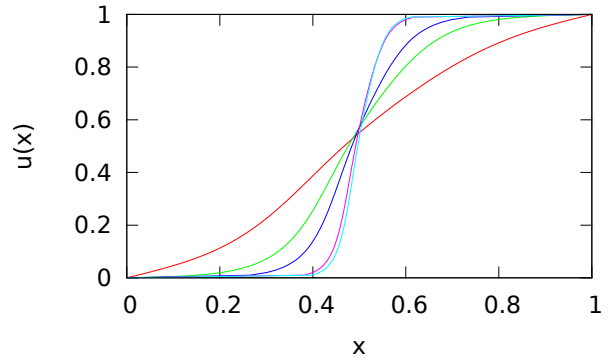


FIG. 8. Graph of the kink for the potential (20) for $a = 1$. The profiles correspond to $k = 3.0, 1.5, 1.0, 0.5, 0.45$ in increasing order of steepness. The two profiles corresponding to $k = 0.5$ and $k = 0.45$ are almost coincident in the picture.

equivalent mechanical system. More precisely, remark that

$$\int_a^b \frac{ds}{\sqrt{2[E + V(s)]}}$$

is an decreasing function of E , defined for $E > 0$, and such that its limit for $E \rightarrow 0$ tends to infinity. Since by (4)

$$\int_a^b \frac{ds}{\sqrt{2[E_k + V(s)]}} = \frac{\ell}{k}$$

it follows that for $k \rightarrow 0$ the energy level E_k tends to 0.

The Theorem 1 is a classical result in interface theory. For the sake of completeness we report the proof in our case.

Proof of Theorem 1. Since V is a strictly positive function in $[u_1, u_2]$, by the dominated convergence theorem it follows immediately that

$$\lim_{k \rightarrow 0} \int_{u_1}^{u_2} \frac{ds}{\sqrt{2[E_k + V(s)]}} = \int_{u_1}^{u_2} \frac{ds}{\sqrt{2V(s)}} < \infty$$

yielding (5). \square

The proof of Theorem 2, based on the heuristic arguments discussed in Section II, uses some ideas developed in [19, Appendix A].

Proof of Theorem 2. Recall the definition (6) of x_k^i . By simple algebra we have that

$$x_k^i = k S_{a,k} + k R_{a,k} \quad (21)$$

where

$$S_{a,k} = \int_a^{\frac{a+b}{2}} \frac{ds}{\sqrt{2[E_k + V''(a)(s-a)^2/2]}}$$

and

$$R_{a,k} = \int_a^{\frac{a+b}{2}} \frac{ds}{\sqrt{2[E_k + V(s)]}} - S_{a,k}$$

By direct integration we get

$$S_{a,k} = \frac{1}{\sqrt{V''(a)}} \operatorname{arcsinh} \left[\sqrt{\frac{V''(a)}{2E_k}} \frac{b-a}{2} \right] \quad (22)$$

The idea behind the proof is the following: once $S_{a,k}$ has been computed explicitly, we are able to manage the divergence of the integral with E_k for $k \rightarrow 0$. On the other hand we shall simply estimate $R_{a,k}$ and prove that it is finite for any $k \geq 0$.

We can perform the analogous computation in the neighborhood of the boundary point ℓ where the bound-

ary condition b has been fixed. Noted that

$$\ell - x_k^i = \int_{\frac{a+b}{2}}^b \frac{k ds}{\sqrt{2[E_k + V(s)]}}$$

we get

$$\ell - x_k^i = k S_{b,k} + k R_{b,k} \quad (23)$$

where

$$\begin{aligned} S_{b,k} &= \int_{\frac{a+b}{2}}^b \frac{ds}{\sqrt{2[E_k + V''(b)(b-s)^2/2]}} \\ &= \frac{1}{\sqrt{V''(b)}} \operatorname{arcsinh} \left[\sqrt{\frac{V''(b)}{2E_k}} \frac{b-a}{2} \right] \end{aligned} \quad (24)$$

and

$$R_{b,k} = \int_{\frac{a+b}{2}}^b \frac{ds}{\sqrt{2[E_k + V(s)]}} - S_{b,k}$$

Recalling that $\operatorname{arcsinh}(x) = \log(x + \sqrt{x^2 + 1})$, by equations (21)–(24) we get

$$\sqrt{V''(a)} x_k^i - \sqrt{V''(b)} (\ell - x_k^i) = k \left[\log \frac{\sqrt{V''(a)}(b-a) + \sqrt{V''(a)(b-a)^2 + 8E_k}}{\sqrt{V''(b)}(b-a) + \sqrt{V''(b)(b-a)^2 + 8E_k}} + \sqrt{V''(a)} R_{a,k} - \sqrt{V''(b)} R_{b,k} \right] \quad (25)$$

which is the analogous of the equation (9) that we obtained in the heuristic discussion in Section II.

By using the explicit expression of $S_{a,k}$ and $S_{b,k}$ we have been able to cancel the divergence in E_k in the first part of the right-hand side of (25). Recall equation (7);

since $E_k \rightarrow 0$ for $k \rightarrow 0$, the theorem will follow from (25) once we shall have proven that

$$\sup_{k \geq 0} |R_{a,k}| < \infty \quad \text{and} \quad \sup_{k \geq 0} |R_{b,k}| < \infty \quad (26)$$

We prove the first of the two bounds above; the second one can be proven similarly. With some algebra we get

$$\begin{aligned} R_{a,k} &= \int_a^{\frac{a+b}{2}} \frac{\sqrt{2E_k + V''(a)(s-a)^2} - \sqrt{2[E_k - V(s)]}}{\sqrt{2E_k + V''(a)(s-a)^2} \sqrt{2[E_k - V(s)]}} ds \\ &= \int_a^{\frac{a+b}{2}} \frac{[-2V(s) + V''(a)(s-a)^2] ds}{\sqrt{2[E_k + V(s)]} [2E_k + V''(a)(s-a)^2] + 2[E_k + V(s)] \sqrt{2E_k + V''(a)(s-a)^2}} \end{aligned}$$

where in the last step we have multiplied numerator and denominator times the sum of the two square root terms.

Since, as we remarked at the beginning of this section, $E_k > 0$ for any $k > 0$ and $E_k \rightarrow 0$ for $k \rightarrow 0$, we have that

$$\sup_{k \geq 0} |R_{a,k}| \leq \int_a^{\frac{a+b}{2}} \frac{|-2V(s) + V''(a)(s-a)^2| ds}{2V(s)\sqrt{V''(a)}(s-a) + \sqrt{2V(s)V''(a)}(s-a)^2}$$

Moreover the integrand is continuous in $(a, (a+b)/2]$ and its limit for $s \rightarrow a$ is $|V'''(a)|/[6V''(a)\sqrt{V''(a)}]$; therefore, we have that the integral on the right-hand side of the inequality above is finite. We thus get the first of the two bounds (26).

As noted below (25) this is sufficient to complete the

proof of the theorem. \square

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